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G-Quadruplexes: A Systematic Investigation on the Interaction of Cations with the Internal Channel Site

Zaccaria, F.

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The structure of G-Quadruplexes (GQs) in DNA were first hypothesized, then experimentally determined, and eventually observed in the genome of animal cells. During the last thirty years, GQ structures have drawn an immense interest in diverse areas, such as structural biology, medicinal chemistry, supramolecular chemistry and nanotechnology.

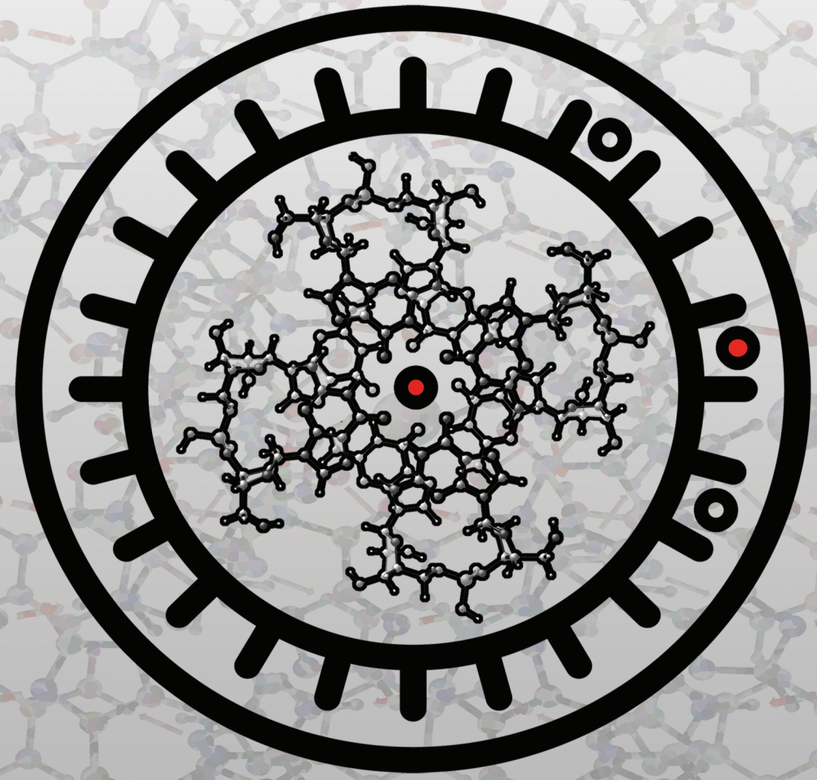
Special focus in this thesis has been dedicated to understanding the interaction between the partially negative internal cavity of the GQ and cations and how the presence of a cation influences the folding of the supramolecular structure.

In the reported investigations, we have leveraged density functional theory to understand and explain the basic physico-chemical rules that govern this interaction. This has allowed us to verify and specify different hypotheses in the literature on the role and necessity of the cations in the internal channel site of G-Quadruplexes.

Francesco Zaccaria graduated in Pharmaceutical Biotechnologies in 2007 at the Federico II University of Napoli. He started his PhD at the VU University of Amsterdam in 2014. Since November 2018 he works as a post-doc researcher for the same university in affiliation with the Italian Institute of Technology in Genova for the development of computational methods in the design of nano-sized semi-conductors.

G-Quadruplexes. Interaction of Cations at the Internal Channel Site F. Zaccaria

G-Quadruplexes. Interaction of Cations at the Internal Channel Site: a Systematic Investigation



Francesco Zaccaria

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